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ON THE NUMERICAL BEHAVIORS OF CUBIC-QUARTIC SPLINE FITS

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1. Introduction

The theories and numerical methods for construction of a spline fits to the data given as horizontal segments, rectangles of uncertainty, and combinations of them with vertical segments, are not well known. The author has studied in [1] a numerical treatment to construct a spline fit from experimental data which are erroneous in two dimensional cartesian coordinate system. Using the general theory of spline functions for fitting, the author has introduced a representation of error on the data in abscissa and ordinate, and found a sufficiently regular function $\sigma(t) \in H^2[a,b]$ (Sobolev space of order 2) such that

$$\begin{aligned}(1.1)\qquad &\int_a^b (\sigma''(t))^2 dt+\rho\sum_{i=1}^n \frac{1}{\varepsilon_i^2}\Big(\frac{1}{b_i-a_i}\int_{a_i}^{b_i}\sigma(t)dt-z_i\Big)^2\\ &=\min_{x\in H^2[a,b]}\Big[\int_a^b (x''(t))^2 dt+\rho\sum_{i=1}^n \frac{1}{\varepsilon_i^2}\Big(\frac{1}{b_i-a_i}\int_{a_i}^{b_i}x(t)dt-z_i\Big)^2\Big]\end{aligned}$$

with $a\leqq a_1\leqq b_1<a_2\leqq b_2<\ldots<a_n\leqq b_n\leqq b$, $\varepsilon_i>0$, $\rho>0$, and $z_i=x(t_i)$. We have deliberated the second term of above expression (1.1) which figures at the same time the error in abscissa represented by $\int_{a_i}^{b_i} x(t)dt/(b_i-a_i)$ where a_i and b_i are the error bounds of the measurement in abscissa $t_i\in[a_i, b_i]=[t_i-\eta_i, t_i+\eta_i]$ with maximum deviation η_i around the measured quantity t_i and the error in ordinate represented by $1/\varepsilon_i^2$ where ε_i measures maximum deviation around the measured quantity z_i. To solve the problem (1.1) we have taken the Hilbert spaces $\mathcal{X}=H^2[a,b]$, $\mathcal{Y}=H^0[a,b]$ and $\mathcal{Z}=\mathbf{R}^n$, and defined the scalar products:

$$\langle k_i|x\rangle_{\mathcal{X}}=\frac{1}{b_i-a_i}\int_{a_i}^{b_i}x(t)dt,\quad \text{for all } x, k_i\in\mathcal{X},$$

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and

$$\langle x|y\rangle_{\mathcal{Z}}=\sum_{i=1}^{n}\frac{1}{\varepsilon_i^2}x_iy_i$$

with $x=(x_1,\dots,x_n)$, $y=(y_1,\dots,y_n)$, and transformed the problem (1.1) into the simple equivalent form introducing the continuous linear operator T of $\mathcal{X}$ into $\mathcal{Y}$ defined by $Tx(t)=x''(t)$ and the mapping A of $\mathcal{X}$ into $\mathcal{Z}$ defined by

$$A(x)=[\langle k_1|x\rangle_{\mathcal{X}},\dots,\langle k_n|x\rangle_{\mathcal{X}}]\in\mathcal{Z}.$$

Using the theorem of the characterization of the best approximation, the author has shown that if $n\geqslant 2$, there exists a unique solution $\sigma(t)$ to the problem (1.1) where n is the number of the given data (see [2]). Such a solution $\sigma(t)$ is called a *cubic-quartic (second order) spline function for fitting*. For the convenience, we suppose that $n\geqslant 3$. Using also the projection method in Hilbert space, we have constructed a theorem which characterizes the solution $\sigma(t)$ to the problem (1.1) as follow:

THOEREM. *The function $\sigma(t)\in\mathcal{X}$ is the cubic-quartic spline function for fitting to the problem* (1.1) (*relatively to T, A, z and $\rho>0$*) *if and only if there exist μ_j $(j=1,\dots,n-2)$ such that*

$$(1.2)\qquad T(\sigma)=\sigma''(t)=\sum_{j=1}^{n-2}\mu_j f^j(t),\ A(\sigma)=z-\frac{1}{\rho}\sum_{j=1}^{n-2}\mu_j b^j.$$

The coefficients μ_j can be obtained by solving the following linear algebraic system of dimension $n-2$

$$(1.3)\qquad \sum_{j=1}^{n-2}\omega_{i,j}\ \mu_j=\langle z|b^j\rangle_{\mathcal{Z}},\quad i=1,\dots,n-2,$$

where $$\omega_{i,j}=\langle f^i(t)\,|\,f^j(t)\rangle_{\mathcal{Y}}+\frac{1}{\rho}\langle b^i|b^j\rangle_{\mathcal{Z}}.$$

In this paper we study on the numerical technique to calculate $\sigma(t)$ practically. We solve first of all the linear algebraic system (1.3) and then determine numerically $\sigma(t)$ from (1.2). With the numerical results we also deliberate on the numerical behaviors of $\sigma(t)$.

2. Numerical solution of the linear algebraic system

Since the matrix $\Omega=(\omega_{i,j})$ is symmetric and pentadiagonal, it is necessary to calculate $f^j(t)$, $f^{j+1}(t)$ and $f^{j+2}(t)$; b_i^j, b_i^{j+1} and b_i^{j+2}. To calculate

$$\langle f^i(t) \mid f^j(t)\rangle_\psi = \int_a^b f^i(t) f^j(t)\,dt, \tag{2.1}$$

it is necessary to examinate precisely the $n-2$ continuous functions $f^j(t)$ $(i=1, \dots, n-2)$ on $[a, b]$ which are defined by the Lemma 2 in [1].

In the case $j=i$, we have

$$\langle f^i(t) \mid f^i(t)\rangle_\psi = \int_{a_i}^{b_i} (f^i(t))^2 dt + \int_{b_i}^{a_{i+1}} (f^i(t))^2 dt + \int_{a_{i+1}}^{b_{i+1}} (f^i(t))^2 dt + \int_{b_{i+1}}^{a_{i+2}} (f^i(t))^2 dt + \int_{a_{i+2}}^{b_{i+2}} (f^i(t))^2 dt.$$

If $a_i \neq b_i$ (*i.e.*, $\eta_i \neq 0$),

$$\int_{a_i}^{b_i} (f^i(t))^2 dt = \int_{a_i}^{b_i} \left\{ \sum_{k=i}^{i+2} \Delta_k^i [(b_i - t)_+^2 - (a_i - t)_+^2] \right\}^2 dt$$

where

$$\Delta_k^i = \frac{1}{2d_k^i (b_i - a_i)}.$$

If $a_i = b_i$ (*i.e.*, $\eta_i = 0$), obviously

$$\int_{a_i}^{b_i} (f^i(t))^2 dt = 0.$$

In the case $j \neq i$, we have

$$\langle f^i(t) \mid f^j(t)\rangle_\psi = \int_{a_i}^{b_i} f^i(t) f^j(t)\,dt + \int_{b_i}^{a_{i+1}} f^i(t) f^j(t)\,dt + \int_{a_{i+1}}^{b_{i+1}} f^i(t) f^j(t)\,dt + \int_{b_{i+1}}^{a_{i+2}} f^i(t) f^j(t)\,dt + \int_{a_{i+2}}^{b_{i+2}} f^i(t) f^j(t)\,dt.$$

REMARK 1. Actually if $a_i \approx b_i$ (*i.e.*. η_i is very small), the coefficients of $f^i(t)$ and $f^j(t)$ are very small. Thus, to calculate $\int_{a_i}^{b_i} (f^i(t))^2 dt$ or $\int_{a_i}^{b_i} f^i(t) f^j(t)\,dt$ numerically, it is preferable to develop at first $(f^i(t))^2$ or $f^i(t) f^j(t)$ to the power form of degree 4 and then to calculate the integrals of each monomials defined in $[a_i, b_i]$.

To calculate

$$\langle b^i \mid b^j\rangle_\varepsilon = \sum_{k=1}^{n} \frac{1}{\varepsilon_k^2} b_k^i b_k^j, \tag{2.2}$$

we get easily b_k^j, b_k^{j+1} and b_k^{j+2} from the definition of b_i^j (confer (4.6) of [1]). Thus we have

$$\langle b^i | b^i \rangle_{\mathcal{Z}} = \sum_{k=i}^{i+2} \frac{1}{\varepsilon_i^2} b_k^i b_k^i$$

$$= \left(\frac{\varepsilon_i}{d_i^i}\right)^2 + \left(\frac{\varepsilon_{i+1}}{d_{i+1}^i}\right)^2 + \left(\frac{\varepsilon_{i+2}}{d_{i+2}^i}\right)^2,$$

$$\langle b^i | b^{i+1} \rangle_{\mathcal{Z}} = \frac{\varepsilon_{i+1}^2}{d_{i+1}^i \cdot d_{i+1}^{i+1}} + \frac{\varepsilon_{i+2}^2}{d_{i+2}^i \cdot d_{i+2}^{i+1}},$$

$$\langle b^i | b^{i+2} \rangle_{\mathcal{Z}} = \frac{\varepsilon_{i+2}^2}{d_{i+2}^i \cdot d_{i+2}^{i+2}}$$

From the results of the calculation (2. 1) and (2. 2), we obtain the *principal diagonal* entries $p_i = \omega_{i,i}$, the *first diagonal* entries $f_i = \omega_{i,i+1} = \omega_{i+1,i}$ and the *second diagonal* entries $s_i = \omega_{i,i+2} = \omega_{i+2,i}$.

We probe the matrix $\Gamma = (\gamma_i)$ such that

$$\gamma_i = \langle z | b^i \rangle_{\mathcal{Z}} = \sum_{k=i}^{i+2} \frac{1}{\varepsilon_k^2} z_k b_k^i.$$

From the n data (the rectangles of uncertainty, the vertical and horizontal segments, and the points), we estimate the vector $z = [z_1, \ldots, z_n] \in \mathcal{Z}$ such that

$$z_i = \frac{c_i + d_i}{2}$$

where $z_i = c_i + \eta_i = d_i - \eta_i$.
From the definition of b_i^j, we know

$$b^i = [o, \ldots, o, b_i^i, b_{i+1}^i, b_{i+2}^i, o, \ldots, o] \in \mathcal{Z}.$$

Consequently,

$$\gamma_i = \langle z | b^i \rangle_{\mathcal{Z}} = \frac{1}{\varepsilon_i^2} z_i b_i^i + \frac{1}{\varepsilon_{i+1}^2} z_{i+1} b_{i+1}^i + \frac{1}{\varepsilon_{i+2}^2} z_{i+2} b_{i+2}^i$$

$$= \frac{z_i}{d_i^i} + \frac{z_{i+1}}{d_{i+1}^i} + \frac{z_{i+2}}{d_{i+2}^i} = \delta_i^2(z),$$

where $\delta_i^2(z)$ designate the operator of divided difference of z on t_i, t_{i+1} and t_{i+2}.

We solve the linear algebraic system (1. 3). Since the n-2 dimensional square matrix Ω is a Gram matrix in $\mathcal{Y} \times \mathcal{Z}$ which is symmetric and positive definite, the existence of the unique solution to the system (1. 3) is guaranteed, and the system (1. 3) is solved by the Gauss method or Choleski method. We should find an algorithm to get the solution vector μ of the system (1. 3). We have already supposed that $n \geqq 3$. When $n=3$, we can get directly. When $n=4$ or 5, we prefer to calculate

μ by the Gauss method because the matrix Ω is of order 2 or 3. When $n \geqq 6$, we use the Choleski method consulting particularly 2. of [5].

REMARK 2. With the Choleski method (i.e., $n \geqq 6$), for the sake of computer memory, the matrix Ω of dimension $(n-2)\times(n-2)$ is stored as the form of a matrix of dimension $(n-2)\times 3$ such that (see [3] and [4]):

$$\begin{pmatrix} p_1 & f_1 & s_1 \\ p_2 & f_2 & s_2 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ p_i & f_i & s_i \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ p_{n-4} & f_{n-4} & s_{n-4} \\ p_{n-4} & f_{n-3} & 0 \\ p_{n-2} & 0 & 0 \end{pmatrix}.$$

3. Numerical determination of cubic-quartic spline fits

To determinethe solution $\sigma(t)$ of the problem (1.1), we estimate at first the conditions $A(\sigma)$. From (1.2) and the definition of the operator A, we have

$$\begin{aligned} (3.1) \qquad A(\sigma) &= z - \frac{1}{\rho}\sum_{j=1}^{n-2}\mu_j b^j \\ &= [\langle k_1 | \sigma\rangle_X, \ldots, \langle k_n | \sigma\rangle_X] \in \mathcal{Z}. \end{aligned}$$

From the Lemma 2 in [1] and (1.2) we obtain also

$$T(\sigma) = \sigma''(t) = \sum_{j=1}^{n-2}\mu_j \sum_{i=j}^{j+2} \Gamma^j(a_i, b_i, t).$$

with
$$\Gamma^j(a_i, b_i, t) = \begin{cases} \dfrac{(b_i - t)_+^2 - (a_i - t)_+^2}{2d_i^j (b_i - a_i)} & \text{if } a_i \neq b_i \\ \dfrac{(t_i - t)_+}{d_i^j} & \text{if } a_i = b_i \end{cases}$$

where

$$d_i^j = \prod_{\substack{l=j \\ i \neq l}}^{j+2} (t_i - t_l), \quad j = 1, \ldots, n-2.$$

Thus, we have

$$\sigma(t)=\sum_{j=1}^{n-2}\mu_j\sum_{i=j}^{j+2}\iint\Gamma^j(a_i, b_i, t)\,dt+At+B$$

where $A$and B are the real constants.
If we let

$$\varphi_i^j(t)=\mu_j\sum_{i=j}^{j+2}\iint\Gamma^j(a_i, b_i, t)\,dt, \quad j=1, \ldots, n-2, \tag{3.2}$$

then

$$\sigma(t)=\sum_{j=1}^{n-2}\varphi_i^j(t)+At+B. \tag{3.3}$$

To calculate A and B together, we take two conditions from (3.1), that is, the first condition $\langle k_1 | \sigma(t)\rangle_\chi$ and the last condition $\langle k_n | \sigma(t)\rangle_\chi$. On the other hand,

$$\langle k_i | \sigma_{2i-1}(t)\rangle_\chi=\frac{1}{b_i-a_i}\int_{a_i}^{b_i}\sigma_{2i-1}(t)\,dt, \quad i=1, \ldots, n,$$

where $\sigma_{2i-1}(t)$ designate the spline fit in $[a_i, b_i]$. Thus the two equations are obtained to calculate A and B as follow:

$$\begin{cases}\langle k_1 | \sigma_1(t)\rangle_\chi=\dfrac{1}{b_1-a_1}\displaystyle\int_{a_1}^{b_1}\sigma_1(t)\,dt,\\ \langle k_n | \sigma_{2n-1}(t)\rangle_\chi=\dfrac{1}{b_n-a_n}\displaystyle\int_{a_n}^{b_n}\sigma_{2n-1}(t)\,dt.\end{cases} \tag{3.4}$$

In each interval $[a_i, b_i]$ or $[b_i, a_{i+1}]$ we calculate the n-2 functions $\varphi_i^j(t)$ of (3.2) with μ_j and determine finally the unique solution $\sigma(t)$ of the problem (1.1) which is cubic-quartic spline function given by (3.3).

REMARK 3. When $a_1=b_1$ or $a_n=b_n$, the system (3.4) has no meaning. If $a_n=b_n$ (i.e. $\eta_n=0$), by the continuity of the $\sigma(t)$, we get an equation

$$\sigma_{2n-2}(t)=\langle k_n | \sigma_{2n-1}(t)\rangle_\chi.$$

Consequently, (3.4) becomes

$$\begin{cases}\langle k_1 | \sigma_1(t)\rangle_\chi=\dfrac{1}{b_1-a_1}\displaystyle\int_{a_1}^{b_1}\sigma_1(t)\,dt,\\ \langle k_n | \sigma_{2n-1}(t)\rangle_\chi=\sigma_{2n-2}(t).\end{cases}$$

If $a_1=b_1$ (i.e. $\eta_1=0$), similarly, (3.4) is transformed

$$\begin{cases}\langle k_1 | \sigma_1(t)\rangle_\chi=\sigma_2(t),\\ \langle k_n | \sigma_{2n-1}(t)\rangle_\chi=\dfrac{1}{b_n-a_n}\displaystyle\int_{a_n}^{b_n}\sigma_{2n-1}(t)\,dt.\end{cases}$$

REMARK 4. In order to solve the linear algebraic system (3. 4), we use the Gauss method. when $b_1=-a_1$, the element of first row and first column of this system is zero. We should then take the pivoting strategy.

4. Numerical behaviors of cubic-quartic spline fits

Having a kind of numerical experiences, we remark the following influences by the change of data and coefficients $\rho_i>0$ of the cubic-quartic spline fits. Some of these remarks are explained theoretically and even numerically.

At first we consider the case of $\varepsilon_i=0$.
From (1. 2) and the definition of b_i^j, $\varepsilon_i=0$ implicates:

(4. 1) Ⅰ) $b_i^j=0$ for all $i=1, \ldots, n-2$, and $\langle k_i|\sigma\rangle=z_i$;
Ⅱ) the coefficients ρ_i have no influence on the spline fits at t_i, that is, all curves of each coefficients ρ_i pass always the same points.

Moreover, if $\eta_i=0$, (4. 1) implicates:
—the value of the spline fit at t_i is z_i.
Therefore the curve pass throughthe points (t_i, z_i).
If $\eta_i\neq 0$, (4. 1) implicates:
—the value of the local integral in $[a_i, b_i]$ equals z_i.
This permits not always that the curve pass through the points (t_i, z_i), but often signify that the curve pass through the neighborhood of the points (t_i, z_i).

On the other hand, with the case of $\varepsilon_i\neq 0$, we get the empirical results such that:

Ⅰ) the ε_i have much more influential than η_i.

Ⅱ) the curve concerned with the greatest coefficients ρ_i pass through the nearest point from the point (t_i, z_i).

Therefore the problem (1. 1) is nicely solved, at least, for a number of constraints which are not very important. Theoretically it is not too difficult to determine the solution $\sigma(t)$. However, it will be desireable to make our method be better to the following directions:

Ⅰ) The generalization to several variables.

Ⅱ) The choice of the proper coefficients $\rho_i>0$ to get optimal result.

Ⅲ) The generalization to the larger order of spline fits.

These seem to be quite possible and are intended to reslove soon or late.

Those who desires to have the computer-programs and the plotting results please contact the author.

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